



ELSEVIER

Computer Physics Communications 91 (1995) 345-347

Computer Physics
Communications

Author index to volume 91

| | |
|--|---------------|
| Antosiewicz, J., see J.D. Madura | 91 (1995) 57 |
| Bagheri, B., see J.D. Madura | 91 (1995) 57 |
| Berendsen, H.J.C., D. van der Spoel and R. van Drunen, GROMACS: A message-passing parallel molecular dynamics implementation | 91 (1995) 43 |
| Briggs, J.M., see J.D. Madura | 91 (1995) 57 |
| Caldwell, J.W., see D.A. Pearlman | 91 (1995) 1 |
| Case, D.A., see D.A. Pearlman | 91 (1995) 1 |
| Cheatham III, T.E., see D.A. Pearlman | 91 (1995) 1 |
| Chow, K.-H. and D.M. Ferguson, Isothermal-isobaric molecular dynamics simulations with Monte Carlo volume sampling | 91 (1995) 283 |
| Daggett, V., see M. Levitt | 91 (1995) 215 |
| Dalke, A., see M. Nelson | 91 (1995) 111 |
| Dauber-Osguthorpe, P., see A.P. Lemon | 91 (1995) 97 |
| Davis, M.E., see J.D. Madura | 91 (1995) 57 |
| DeBolt, S., see D.A. Pearlman | 91 (1995) 1 |
| Elber, R., A. Roitberg, C. Simmerling, R. Goldstein, H. Li, G. Verkhivker, C. Keasar, J. Zhang and A. Ulitsky, MOIL: A program for simulations of macromolecules | 91 (1995) 159 |
| Endo, S., see H. Wako | 91 (1995) 233 |
| Ferguson, D., see D.A. Pearlman | 91 (1995) 1 |
| Ferguson, D.M., see K.-H. Chow | 91 (1995) 283 |
| Gilson, M.K., see J.D. Madura | 91 (1995) 57 |
| Gō, N., see H. Wako | 91 (1995) 233 |
| Goldstein, R., see R. Elber | 91 (1995) 159 |
| Goodfellow, J.M., W.R. Pitt, O.S. Smart and M.A. Williams, New methods for the analysis of the protein-solvent interface | 91 (1995) 321 |
| Guilbert, C., D. Perahia and L. Mouawad, A method to explore transition paths in macromolecules. Applications to hemoglobin and phosphoglycerate kinase | 91 (1995) 263 |
| Gursoy, A., see M. Nelson | 91 (1995) 111 |
| Hirshberg, M., see M. Levitt | 91 (1995) 215 |
| Humphrey, W., see M. Nelson | 91 (1995) 111 |
| Hünenberger, P.H., see W.F. van Gunsteren | 91 (1995) 305 |

- Ilin, A., see J.D. Madura 91 (1995) 57
- Kale, L., see M. Nelson 91 (1995) 111
- Keasar, C., see R. Elber 91 (1995) 159
- Keiner, V., see G.R. Kneller 91 (1995) 191
- Kneller, G.R., V. Keiner, M. Kneller and M. Schiller, *nMOLDYN*: A program package for a neutron scattering oriented analysis of molecular dynamics simulations 91 (1995) 191
- Kneller, M., see G.R. Kneller 91 (1995) 191
- Kollman, P., see D.A. Pearlman 91 (1995) 1
- Kufrin, R., see M. Nelson 91 (1995) 111
- Lavery, R., K. Zakrzewska and H. Sklenar, JUMNA (Junction minimisation of nucleic acids) 91 (1995) 135
- Lemon, A.P., P. Dauber-Osguthorpe and D.J. Osguthorpe, FOCUS: a molecular dynamics analysis program. New features for the characterisation of lipid bilayers and solvated systems 91 (1995) 97
- Levitt, M., M. Hirshberg, R. Sharon and V. Daggett, Potential energy function and parameters for simulations of the molecular dynamics of proteins and nucleic acids in solution 91 (1995) 215
- Li, H., see R. Elber 91 (1995) 159
- Luty, B.A., see J.D. Madura 91 (1995) 57
- McCammon, J.A., see J.D. Madura 91 (1995) 57
- Madura, J.D., J.M. Briggs, R.C. Wade, M.E. Davis, B.A. Luty, A. Ilin, J. Antosiewicz, M. K. Gilson, B. Bagheri, L.R. Scott and J.A. McCammon, Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian Dynamics program 91 (1995) 57
- Mark, A.E., see W.F. van Gunsteren 91 (1995) 305
- Micu, A.M. and J.C. Smith, SERENA: a program for calculating X-ray diffuse scattering intensities from molecular dynamics trajectories 91 (1995) 331
- Mouawad, L., see C. Guilbert 91 (1995) 263
- Nagayama, K., see H. Wako 91 (1995) 233
- Nelson, M., W. Humphrey, R. Kufrin, A. Gursoy, A. Dalke, L. Kale, R. Skeel and K. Schulten, MDScope—a visual computing environment for structural biology 91 (1995) 111
- Osguthorpe, D.J., see A.P. Lemon 91 (1995) 97
- Pearlman, D.A., D.A. Case, J.W. Caldwell, W.S. Ross, T.E. Cheatham III, S. DeBolt, D. Ferguson, G. Seibel and P. Kollman, AMBER, a package of computer programs for applying molecular mechanics, normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules 91 (1995) 1
- Perahia, D., see C. Guilbert 91 (1995) 263
- Perahia, D., see T. Simonson 91 (1995) 291
- Pettitt, B.M., see P.E. Smith 91 (1995) 339
- Pitt, W.R., see J.M. Goodfellow 91 (1995) 321
- Roitberg, A., see R. Elber 91 (1995) 159
- Ross, W.S., see D.A. Pearlman 91 (1995) 1
- Roux, B., The calculation of the potential of mean force using computer simulations 91 (1995) 275

- Schiller, M., see G.R. Kneller 91 (1995) 191
- Schulten, K., see M. Nelson 91 (1995) 111
- Scott, L.R., see J.D. Madura 91 (1995) 57
- Seibel, G., see D.A. Pearlman 91 (1995) 1
- Sharon, R., see M. Levitt 91 (1995) 215
- Simmerling, C., see R. Elber 91 (1995) 159
- Simonson, T. and D. Perahia, Dielectric properties of proteins from simulations: tools and techniques 91 (1995) 291
- Skeel, R., see M. Nelson 91 (1995) 111
- Sklenar, H., see R. Lavery 91 (1995) 135
- Smart, O.S., see J.M. Goodfellow 91 (1995) 321
- Smith, J.C., see A.M. Micu 91 (1995) 331
- Smith, P.E., see W.F. van Gunsteren 91 (1995) 305
- Smith, P.E. and B.M. Pettitt, Efficient Ewald electrostatic calculations for large systems 91 (1995) 339
- Tironi, I.G., see W.F. van Gunsteren 91 (1995) 305
- Ulitsky, A., see R. Elber 91 (1995) 159
- Van Belle, D. and S.J. Wodak, Extended Lagrangian formalism applied to temperature control and electronic polarization effects in molecular dynamics simulations 91 (1995) 253
- Van Drunen, R., see H.J.C. Berendsen 91 (1995) 43
- Van der Spoel, D., see H.J.C. Berendsen 91 (1995) 43
- Van Gunsteren, W.F., P.H. Hünenberger, A.E. Mark, P.E. Smith and I.G. Tironi, Computer simulation of protein motion 91 (1995) 305
- Verkhivker, G., see R. Elber 91 (1995) 159
- Wade, R.C., see J.D. Madura 91 (1995) 57
- Wako, H., S. Endo, K. Nagayama and N. Gō, FEDER/2: program for static and dynamic conformational energy analysis of macro-molecules in dihedral angle space 91 (1995) 233
- Williams, M.A., see J.M. Goodfellow 91 (1995) 321
- Wodak, S.J., see D. Van Belle 91 (1995) 253
- Zakrzewska, K., see R. Lavery 91 (1995) 135
- Zhang, J., see R. Elber 91 (1995) 159